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We show that different conventions for Bloch Hamiltonians on non-Bravais lattices correspond to different natural definitions of parallel transport of Bloch eigenstates. Generically the Berry curvatures associated with these parallel transports differ, while physical quantities are naturally related to a canonical choice of the parallel transport.

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An increasing effort has been recently devoted to the characterization of geometrical and topological properties of electronic bands in crystals. Several physical concepts, including the semi-classical evolution and the polarizability, were related through the geometrical notions of Berry connection, curvature, and phase to the parallel transport within electronic bands [1–4]. It was recently proposed to experimentally access such Berry properties in cold atoms lattices [5, 6]. Blount already noted [7] that a quantity analogous to an electromagnetic vector potential characterizes isolated bands in a crystal. With the advent of the integer quantum Hall effect, the first Chern class of electronic bands was described via a connection defining parallel transport of eigenstates over the Brillouin zone [8]. Independently, Berry [1] introduced a similar notion of parallel transport to describe the adiabatic evolution of eigenstates of a time dependent Hamiltonian. Both notions of parallel transport were related soon after [9], and the properties of parallel transport of eigenstates in crystals are now associated with a Berry connection, although they are not necessarily related to a Hamiltonian adiabatic evolution.

Electronic eigenstates in a crystal can be deduced from a Bloch Hamiltonian depending on a quasi-momentum in the Brillouin zone [7]. However, as noted by Zak, this Hamiltonian does not have a unique matrix form for a given model on a crystal [10]. Several conventions exist for bases of Bloch states over the Brillouin zone, as recently discussed in the context of graphene-like systems in [11, 12]. Such different conventions define different ways of transporting eigenstates parallel to the bases. The different parallel transports do not necessarily define unique "Berry geometrical properties" when restricted to a (few) band(s). It is the purpose of this paper to show that different "Berry curvatures" are obtained out of commonly used Bloch conventions for models defined on non-Bravais lattices such as graphene. Moreover, we point to a canonical Bloch convention that allows to define parallel transport in an (almost) unambiguous way. When projected on a (few) band(s), the latter defines the physically relevant "Berry connection" characterizing measurable properties of the crystal. The above situation differs from the Hamiltonian adiabatic evolution initially considered by Berry where the parallel transport in the whole Hilbert space is unambiguously defined from the start.

Let us begin by considering a crystal $\mathcal{C}$, a discrete subset of a d-dimensional Euclidean space E^d (the locations of atoms) acted upon by a Bravais lattice $\Gamma \subset \boldsymbol{R}^d$ of discrete translations, $\Gamma \simeq \boldsymbol{Z}^d$. For non-Bravais crystals, several classes of translationally equivalent points of $\mathcal{C}$ called sublattices exist: the cardinal N of $\mathcal{C}/\Gamma$ is larger than 1. For example, the hexagonal lattice of graphene possesses $N = 2$ sublattices A and B marked, respectively, as full and empty circles in the insets of Fig. 1. The Bravais lattice is composed of vectors connecting sites of the same sublattice. The set $\mathcal{C}/\Gamma$ may be represented by a fundamental domain $\mathcal{F} \subset \mathcal{C}$, also called a unit cell, which has one point in each sublattice. A translation of $\mathcal{F}$ by a Bravais vector is also a possible choice for a unit cell but when $N > 1$ then there are choices of $\mathcal{F}$ that are not related in this way. Two such choices for graphene are illustrated in the insets of Fig. 1a and b.

Along with the translational degrees of freedom, one may consider a finite number of internal degrees of freedom of atoms, e.g. the spin of electrons, represented as a finite-dimensional complex vector space V equipped with a scalar product $\langle\cdot,\cdot\rangle_V$. The Hilbert space of crystalline states is then the space $\boldsymbol{H} = \ell^2(\mathcal{C}, V)$ of V-valued square-summable functions on $\mathcal{C}$ with the scalar product $\langle\psi|\chi\rangle = \sum_{x\in\mathcal{C}}\langle\psi(x)|\chi(x)\rangle_V$. The translation of states $\psi \in \boldsymbol{H}$ by a vector γ of the Bravais lattice is defined by the unitary operator T_γ such that $T_\gamma\psi(x) = \psi(x-\gamma)$ for $x \in \mathcal{C}$. Below, we shall assume for simplicity that $V = \boldsymbol{C}$ but all considerations generalize in a straightforward way to the case with internal degrees of freedom.

Operators T_γ define a representation of the translation group Γ in $\boldsymbol{H}$ which may be decomposed into irreducible 1-dimensional components. Irreducible representations of Γ are its characters $\gamma \mapsto \mathrm{e}^{\mathrm{i}k\cdot\gamma}$, where $k \in \boldsymbol{R}^d$. As $\mathrm{e}^{\mathrm{i}k\cdot\gamma} = \mathrm{e}^{\mathrm{i}(k+G)\cdot\gamma}$ for G in the reciprocal lattice $\Gamma^\star$ (composed of vectors G with $G\cdot\gamma \in 2\pi\boldsymbol{Z}$), the characters of Γ form a d-dimensional Brillouin torus $\mathrm{BZ} = \boldsymbol{R}^d/\Gamma^\star$. The decomposition of $\boldsymbol{H}$ into irreducible components is realized by the Fourier transform $\psi \mapsto \widehat{\psi}$, where

$$\widehat{\psi}_k(x) = \sum_{\gamma\in\Gamma} \mathrm{e}^{-\mathrm{i}k\cdot\gamma}\psi(x-\gamma). \tag{1}$$

Note that $\widehat{\psi}_k = \widehat{\psi}_{k+G}$ and

$$\widehat{\psi}_k(x-\gamma) = \mathrm{e}^{\mathrm{i}k\cdot\gamma}\widehat{\psi}_k(x) \tag{2}$$

so that $\widehat{T_\gamma\psi}_k(x) = \mathrm{e}^{\mathrm{i}k\cdot\gamma}\widehat{\psi}_k(x)$. Property (2) defines the Bloch functions on $\mathcal{C}$ with quasi-momentum k. For fixed k, such functions $\varphi_k(x)$ form a finite-dimensional space $\mathcal{H}_k = \mathcal{H}_{k+G}$ that may be equipped with the scalar product $\langle\varphi_k|\chi_k\rangle_k = \sum_{\mathcal{C}/\Gamma}\overline{\varphi_k(x)}\chi_k(x)$. As a Bloch function is determined by its values on a unit cell $\mathcal{F}\subset\mathcal{C}$, $\dim(\mathcal{H}_k) = N$. Note that spaces $\mathcal{H}_k$ are defined canonically for each k, without any further choices.

Geometrically, the collection of vector spaces $\mathcal{H}_k$ forms a complex N-dimensional vector bundle $\mathcal{H}$ over the Brillouin torus BZ. We shall call $\mathcal{H}$ the Bloch bundle. Spaces $\mathcal{H}_k$ are the fibers of $\mathcal{H}$ and their scalar product equips $\mathcal{H}$ with a Hermitian structure. Sections of $\mathcal{H}$ are maps $k\mapsto\varphi_k\in\mathcal{H}_k$. They are smooth if functions $k\mapsto\varphi_k(x)$ are smooth for all x. The Fourier transform (1) is an isomorphism between $\boldsymbol{H}$ and the space of square-integrable sections $k\mapsto\widehat{\psi}_k$ of the Bloch bundle $\mathcal{H}$ defined over BZ. It preserves the norm, as stated by the Plancherel formula. Its inverse is given by the normalized integral of $\widehat{\psi}_k(x)$ over the Brillouin torus.

To compare vectors in different fibers along a curve in the base space of a bundle one needs a parallel transport, as in the Bloch bundle where fibers $\mathcal{H}_k$ are distinct vector spaces for different k. Such a transport is usually not given *a priori* and requires a prescription, provided by a so-called connection. Equivalently, a covariant derivative of sections encodes infinitesimal parallel transport along coordinate axes in the base space. Connections always exist, in particular in the Bloch bundle, but are non-unique and may be non-flat in the sense that the parallel transport of a state along a closed loop does not end in the same state even if the loop may be continuously deformed to a point. Only special bundles carry flat connections. The Bloch bundle does because it may be trivialized (but not in a canonical way). A trivialization of $\mathcal{H}$ is a family of smooth sections $k\mapsto e^i_k$, $i=1,\dots,N$, defined over BZ (i.e. with $e^i_k = e^i_{k+G}$), which for each k form an orthonormal basis (a *frame*) of $\mathcal{H}_k$. An example of a trivialization of $\mathcal{H}$ is provided by the Fourier transforms of functions δ_{x,x_i} concentrated at points x_i, $i=1,\dots,N$, of a fixed unit cell $\mathcal{F}\subset\mathcal{C}$. We shall denote by $e^{\mathrm{I}i}_k$ the corresponding vectors in $\mathcal{H}_k$. Bloch functions decompose as $\varphi_k = \sum_i\varphi_k(x_i)e^{\mathrm{I}i}_k$. The trivialization of $\mathcal{H}$ defined this way depends on the choice of $\mathcal{F}$. If $\mathcal{F}'$ is another unit cell then $x'_i = x_i+\gamma_i$ with $\gamma_i\in\Gamma$ for an appropriate numbering of its points so that $\delta_{x,x'_i} = T_{\gamma_i}\delta_{x,x_i}$ and, consequently, $e'^{\mathrm{I}i}_k = \mathrm{e}^{\mathrm{i}k\cdot\gamma_i}e^{\mathrm{I}i}_k$.

Each trivialization permits to identify the Bloch bundle $\mathcal{H}$ with the trivial bundle $\mathrm{BZ}\times\boldsymbol{C}^N$ and to equip $\mathcal{H}$ with a flat connection that we identify with the covariant derivative $\nabla = \sum dk_\mu\nabla_\mu$ acting on smooth sections $k\mapsto\varphi_k$ of $\mathcal{H}$ by the formula

$$\langle e^i_k|\nabla\varphi_k\rangle_k = d\langle e^i_k|\varphi_k\rangle_k \tag{3}$$

where $d = \sum dk_\mu\partial_\mu$ is the exterior derivative of functions on BZ. Flatness of the connection means that $\nabla^2 = 0$. It follows from the property $d^2=0$ of the exterior derivative. We shall denote by ∇^{I} the flat connection associated to the trivialization $k\mapsto e^{\mathrm{I}i}_k$ of $\mathcal{H}$ defined above. ∇^{I} depends on the choice of unit cell $\mathcal{F}$ but is independent of the numbering of its points. For another unit cell $\mathcal{F}'$ related to $\mathcal{F}$ as discussed above, we have $\nabla'^{\mathrm{I}} = \nabla^{\mathrm{I}} - \mathrm{i}\sum_i|e^{\mathrm{I}i}_k\rangle\langle e^{\mathrm{I}i}_k|\,dk\cdot\gamma_i$. The difference is a differential 1-form with values in linear transformations of the fibers of $\mathcal{H}$.

There exists a more canonical and physically more relevant way to equip the Bloch bundle with a flat connection. Upon a choice of the origin x_0 in the Euclidean space E^d, we may identify Bloch functions with Γ-periodic functions on $\mathcal{C}$ by writing for any $\varphi_k\in\mathcal{H}_k$,

$$\varphi_k(x) = \mathrm{e}^{-\mathrm{i}k\cdot(x-x_0)}u_k(x). \tag{4}$$

Clearly $u_k(x+\gamma) = u_k(x)$ and $u_{k+G}(x) = \mathrm{e}^{\mathrm{i}G\cdot(x-x_0)}u_k(x)$ for $\gamma\in\Gamma$ and $G\in\Gamma^\star$. This allows to identify the Bloch bundle with the quotient of the trivial bundle $\boldsymbol{R}^d\times\ell^2(\mathcal{C}/\Gamma)$ over $\boldsymbol{R}^d$, with the fiber composed of Γ-periodic functions $u(x)$ on $\mathcal{C}$, by the action

$$(k,u(x))\longmapsto(k+G,\,\mathrm{e}^{\mathrm{i}G\cdot(x-x_0)}u(x)) \tag{5}$$

of the reciprocal lattice $\Gamma^\star$. Note that an element $G\in\Gamma^\star$ acts on $u(x)$ by multiplying it by the Γ-periodic function $\mathrm{e}^{\mathrm{i}G\cdot(x-x_0)}$, preserving the $\ell^2(\mathcal{C}/\Gamma)$ scalar product. The trivial bundle $\boldsymbol{R}^d\times\ell^2(\mathcal{C}/\Gamma)$ has a natural flat connection given by the exterior derivative of its sections. As the functions $\mathrm{e}^{\mathrm{i}G\cdot(x-x_0)}$ do not depend on k, this connection commutes with the action of $\Gamma^\star$ and, consequently, it induces a connection ∇^{II} on the Bloch bundle $\mathcal{H}$. The induced connection is still flat: $(\nabla^{\mathrm{II}})^2=0$, but it has a non-trivial holonomy along the non-contractible loops of the Brillouin torus BZ. This holonomy may be identified via relation (4) with the above action of $\Gamma^\star$ on $\ell^2(\mathcal{C}/\Gamma)$. Physical importance of connection ∇^{II} resides in the fact that $-\mathrm{i}\nabla^{\mathrm{II}}_\mu$ corresponds under the Fourier transform to the position operator multiplying wave functions $\psi(x)$ by $(x-x_0)_\mu$. We can still use eq. (3) to define ∇^{II} but now with Bloch functions $e^i_k(x) = \mathrm{e}^{-\mathrm{i}k\cdot(x-x_0)}u^i(x)$, where u^i, $i=1,\dots,N$, form any orthonormal basis of the space $\ell^2(\mathcal{C}/\Gamma)$ of Γ-periodic functions on $\mathcal{C}$ (note that $e^i_{k+G}\neq e^i_k$ in this case). For the particular choice with $u^i(x) = \sum_{\gamma\in\Gamma}T_\gamma\delta_{x,x_i}$, where x_i are the points of a unit cell $\mathcal{F}$, we shall denote the corresponding Bloch functions by $e^{\mathrm{II}i}_k(x)$. Although connection ∇^{II} does not depend on the choice of $\mathcal{F}$, it does depend on the choice of the origin x_0 of the Euclidean space, but in a very simple way. If we choose another origin x'_0 then $e'^{\mathrm{II}i}_k = \mathrm{e}^{\mathrm{i}k\cdot(x'_0-x_0)}e^{\mathrm{II}i}$ so that $\nabla'^{\mathrm{II}} = \nabla^{\mathrm{II}} - \mathrm{i}\,dk\cdot(x'_0-x_0)$, i.e. the two connections differ

by a closed scalar 1-form. To compare connections $\nabla^{\rm I}$ and $\nabla^{\rm II}$, one notes that $e^{{\rm II}i}_k = {\rm e}^{-{\rm i}k\cdot(x_i-x_0)}e^{{\rm I}i}_k$ for the same choice of $\mathcal{F}$. Hence $\nabla^{\rm II} = \nabla^{\rm I} - {\rm i}\sum_i |e^{{\rm I}i}_k\rangle\langle e^{{\rm I}i}_k|\, dk\cdot(x_i - x_0)$.

Often we restrict our attention to electronic states in a Γ-invariant subspace of $\boldsymbol{H}$, such as valence bands in an insulator. This amounts to consider a subbundle $\mathcal{E}$ of the Bloch bundle, *i.e.* a collection of M-dimensional vector subspaces $\mathcal{E}_k \subset \mathcal{H}_k$ smoothly dependent on k and such that $\mathcal{E}_{k+G} = \mathcal{E}_k$. Any connection ∇ on the bundle $\mathcal{H}$ projects to a connection ${}^{\mathcal{E}}\nabla$ on $\mathcal{E}$ for which the covariant derivative of sections $k \mapsto \varphi_k \in \mathcal{E}_k$ is given by

$$ {}^{\mathcal{E}}\nabla\varphi_k = \mathcal{P}_k\nabla\varphi_k \tag{6}$$

where $\mathcal{P}_k$ is the orthogonal projector from $\mathcal{H}_k$ to $\mathcal{E}_k$. In general, flat connections project to connections with curvature. In particular, if ∇ is a flat connection obtained by formula (3) then $\langle e^i_k|{}^{\mathcal{E}}\nabla\varphi_k\rangle_k = \sum_j P^{ij}_k d\langle e^j_k|\varphi_k\rangle_k$ where $P^{ij}_k = \langle e^i_k|\mathcal{P}_k|e^j_k\rangle_k$. In this case

$$ \langle e^i_k|{}^{\mathcal{E}}\nabla^2\varphi_k\rangle_k = \sum_j F^{ij}_k\langle e^j_k|\varphi_k\rangle_k \tag{7}$$

where $F^{ij} = \sum_{mn} P^{im}dP^{mn}\wedge dP^{nj}$ is the matrix curvature 2-form and $F = \sum_i F^{ii} = {\rm tr}\,(PdP\wedge dP)$ is its scalar version.

The integrals divided by $-2\pi{\rm i}$ of F over 2-dimensional (sub-tori in) BZ give the 1st Chern number(s) of the vector bundle $\mathcal{E}$ that are independent of the choice of connection. We may work, in particular, with the connections ${}^{\mathcal{E}}\nabla^{\rm I}$ or ${}^{\mathcal{E}}\nabla^{\rm II}$ obtained by projection of $\nabla^{\rm I}$ and $\nabla^{\rm II}$ to $\mathcal{E}$. Scalar curvature $F^{\rm I}$ corresponding to connection ${}^{\mathcal{E}}\nabla^{\rm I}$ depends in general on the unit cell $\mathcal{F}\subset\mathcal{C}$ whereas scalar curvature $F^{\rm II}$ corresponding to connection ${}^{\mathcal{E}}\nabla^{\rm II}$ does not depend on x_0 and is canonically defined for each subbundle $\mathcal{E}\subset\mathcal{H}$. To see this note that the difference between different frames of sections $k\mapsto e^i_k$ and $k\mapsto e'^i_k$ involved in the definitions (3) has the form $e^i_k = \sum_j U^{ji}_k e'^j_k$ for unitary matrices U_k. The corresponding projectors P'_k and P_k given by matrices P'^{ij}_k and P^{ij}_k are related by the equality $P'_k = U_kP_kU_k^{-1}$ leading to the relation

$$ F' = F + {\rm tr}\,(dP\wedge U^{-1}dU - P\,U^{-1}dU\wedge U^{-1}dU). \tag{8}$$

In general, operators U do not commute with P and we obtain different scalar curvatures. An exception is the relation between the sections $k\mapsto e^{{\rm II}i}_k$ corresponding to different x_0 where operators U are scalar and $P' = P$ resulting in the same scalar curvatures.

We shall use the above geometric setup for the case of the subbundle $\mathcal{E}\subset\mathcal{H}$ of the valence-band states of an insulator. To this end, let us consider a tight-binding Hamiltonian

$$ H = \sum_{x,y\in\mathcal{C}} h_{x,y}|x\rangle\langle y| \tag{9}$$

in the Hilbert space $\boldsymbol{H}$, where $|y\rangle$ denotes the state with localized wave function $x\mapsto\delta_{x,y}$. We shall assume that $h_{x,y} = \overline{h_{y,x}}$ vanishes for $|x-y|$ outside some fixed range. If $h_{x,y} = h_{x+\gamma,y+\gamma}$ for $\gamma\in\Gamma$ then H commutes with Bravais lattice translations T_γ and maps Bloch functions into Bloch functions, defining Bloch Hamiltonians $H_k = H_{k+G}$ acting in the finite-dimensional spaces $\mathcal{H}_k$. Under the Fourier transform (1),

$$ \widehat{H\psi}_k = H_k\widehat{\psi}_k. \tag{10}$$

Given a frame of sections $k\mapsto e^i_k$ of the Bloch bundle $\mathcal{H}$, Hamiltonians H_k may be represented by $N\times N$ Bloch matrices $\langle e^i_k|H_k|e^j_k\rangle_k \equiv H^{ij}_k = \overline{H^{ji}_k}$ related by unitary transformations for different choices of the frame but describing the same physics. In particular, we may obtain Bloch matrices $H^{\rm I}_k = H^{\rm I}_{k+G}$ corresponding to the choice of frames $e^{{\rm I}i}_k$ or $H^{\rm II}_k \neq H^{\rm II}_{k+G}$ corresponding to the frames $e^{{\rm II}i}_k$, a situation considered in [13]. These matrices are the usual standard forms of Bloch Hamiltonians. In the context of graphene, they correspond to the two conventions discussed in [12]. The spectrum $E_{k1}\leq\cdots\leq E_{kN}$ of the Bloch matrices is independent of the frame and coincides with the spectrum of operators H_k. For insulators, the Fermi energy ϵ_F has a value that lies in the spectral gap, i.e. it differs from all E_{kn}. The subspaces $\mathcal{E}_k\subset\mathcal{H}_k$ corresponding to $E_{kn}<\epsilon_F$ form the valence-band subbundle $\mathcal{E}$ of the Bloch bundle $\mathcal{H}$. The space of sections of $\mathcal{E}$ is mapped by the inverse Fourier transform to the subspace $\boldsymbol{E}\subset\boldsymbol{H}$ of the electronic states with energy $<\epsilon_F$ that are filled at zero-temperature. The geometrical properties of bundle $\mathcal{E}$ have a bearing on the low temperature physics of the insulator. The previous discussion applies directly to the valence-band subbundle. In particular, we may equip $\mathcal{E}$ with different connections ${}^{\mathcal{E}}\nabla^{\rm I}$ or ${}^{\mathcal{E}}\nabla^{\rm II}$ whose scalar curvatures differ but give rise to the same Chern numbers.

We can express the projected connections ${}^{\mathcal{E}}\nabla$ in terms of a local frame $k\mapsto\varphi^a_k = \sum_i\varphi^a_i e^i_k$, $a=1,\ldots,M$, of $\mathcal{E}$, *e.g.* composed of the eigenstates of Hamiltonians H_k with energies $E_{ka}<\epsilon_F$ over regions in BZ where no such energy levels cross. For ∇ given by (3), one has:

$$ \langle\varphi^a_k|{}^{\mathcal{E}}\nabla\varphi^b_k\rangle_k = \sum_i\overline{\varphi^a_{ki}}d\varphi^b_{ki} \equiv A^{ab}_k \tag{11}$$

where $A^{ab} = -\overline{A^{ba}}$ is the local connection 1-form, and $F = \sum_a dA^{aa}$. The same relation defines the *Berry connection* extracted from the change of eigenstates under adiabatic changes of the Hamiltonian. Although there is usually no underlying physical adiabatic process involved in the definition of connections projected on the valence-band subbundle, those are often dubbed "Berry connections". We may just talk of Berry connections ${}^{\mathcal{E}}\nabla^{\rm I}$ and ${}^{\mathcal{E}}\nabla^{\rm II}$ on $\mathcal{E}$. In particular, the (almost) canonical connection ${}^{\mathcal{E}}\nabla^{\rm II}$ is related to the position operator projected on the subspace $\boldsymbol{E} = P^-\boldsymbol{H}$ of states with energy $<\epsilon_F$: the operator $(x-x_0)^-_\mu \equiv P^-(x-x_0)_\mu P^-$ corresponds under the Fourier

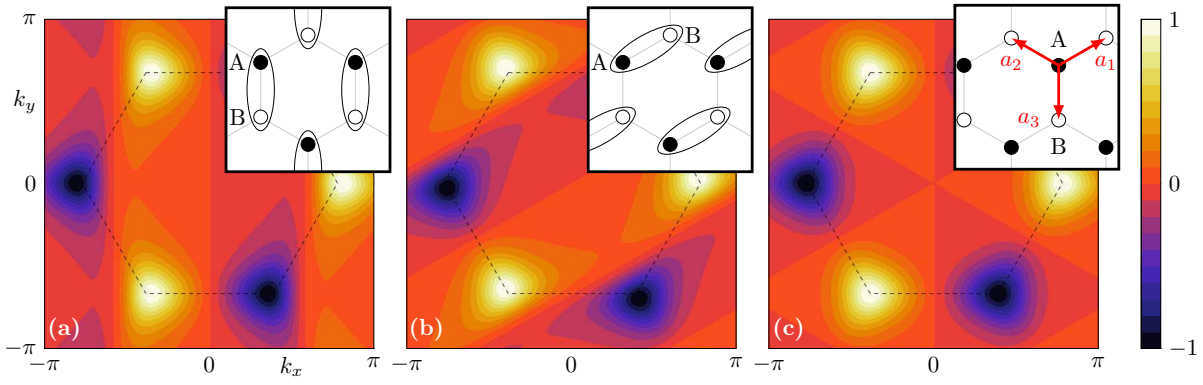

FIG. 1. The (normalized) Berry curvature F_k of the valence band in a gapped graphene model (12) with $v/t = 1$ is plotted on the Brillouin zone (dashed hexagone) for conventions I (a and b) and II (c). The corresponding choices of unit cells for convention I are shown in the insets. Vectors a_i connecting nearest neighbors in sublattices A and B of the graphene lattice are shown in inset (c). In all three cases, curvature F_k is concentrated around the Dirac points of graphene. It depends strongly on the unit cell for convention I and is uniquely defined and respects the symmetries of the crystal for convention II.

transform to the covariant derivative $-\mathrm{i}^{\mathcal{E}}\nabla^{\mathrm{II}}_\mu$ and, for a single valence band, the commutator $[(x-x_0)^-_\mu, (x-x_0)^-_\nu]$ measuring the non-commutativity of the projected position operators corresponds to the multiplication by the component $F^{\mathrm{II}}_{\nu\mu}$ of the canonical scalar curvature F^{II}. One may trace back the occurrence of Berry connection ∇^{II} in physical properties [3, 4] to the above relations.

We now illustrate the different choices of Berry connections on the gapped graphene model with an alternate potential on different sublattices. The model is described by the Hamiltonian

$$H = t\sum_{\langle x,y\rangle} |x\rangle\langle y| + \sum_{x\in\mathcal{C}} v_x |x\rangle\langle x| \qquad (12)$$

where $\langle x, y\rangle$ run through the nearest neighbor pairs on the hexagonal crystal $\mathcal{C}$ and $v_x = +v$ (resp. $-v$) on its sublattice A (resp. B). In convention I, for the unit cell $\mathcal{F} = \{x_A, x_B\}$ shown in Fig. 1a, the Bloch matrix Hamiltonians are

$$H^{\mathrm{I}}_k = \begin{pmatrix} +v & \overline{g^{\mathrm{I}}_k} \\ g^{\mathrm{I}}_k & -v \end{pmatrix} \qquad (13)$$

with $g^{\mathrm{I}}_k = t[1 + \exp(\mathrm{i}k\cdot b_1) + \exp(-\mathrm{i}k\cdot b_2)]$, where $b_i = \varepsilon_{ijk}(a_j - a_k)$ are the Bravais vectors between second-nearest neighbors and a_i, $i = 1, 2, 3$, the ones between nearest neighbors shown on the inset in Fig. 1c. A second choice of unit cell $\mathcal{F}'$ shown in Fig. 1b leads to $g'^{\mathrm{I}}_k = t[1 + \exp(\mathrm{i}k\cdot b_2) + \exp(-\mathrm{i}k\cdot b_3)]$. These Hamiltonians are periodic in k but they explicitly depend on the choice of unit cell. The Hamiltonians H^{II}_k in canonical convention II can be deduced from H^{I}_k using the change of basis matrix $U_k = \mathrm{e}^{\mathrm{i}k\cdot x_0}\,\mathrm{diag}(\mathrm{e}^{-\mathrm{i}k\cdot x_A}, \mathrm{e}^{-\mathrm{i}k\cdot x_B})$ with an arbitrary x_0. It takes the form (13) but with g^I_k replaced by $g^{\mathrm{II}}_k = \mathrm{e}^{\mathrm{i}k\cdot a_3} g^{\mathrm{I}}_k = t[\exp(\mathrm{i}k\cdot a_1) + \exp(\mathrm{i}k\cdot a_2) + \exp(\mathrm{i}k\cdot a_3)]$. In all cases the spectrum is $E_{k\pm} = \pm(v^2 + |g_k|^2)^{1/2}$ and, for $\epsilon_F = 0$, the valence band corresponds to the minus sign. Curvature F of the valence-band subbundle has only one component F_{12}. It is represented in Fig. 1 for the three above conventions for the gapped graphene with unit v/t. The dependence of the Berry curvature on the Bloch conventions is clearly illustrated. In particular, for convention I, a rotation of the unit cell rotates the curvature plot while a translation of the unit cell amounts to a $U(1)$ gauge transformation and does not change the curvature.

This ends our discussion of the two main conventions used to define Berry connections in subbundles of Bloch states, the main subject of the present paper. We showed how in one of those conventions the scalar curvature depends on additional choices and we identified another, more physical, convention in which the scalar curvature is unambiguously defined and relates to the position operator.

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